Linalool oxide acetate

Inchi: InChI=1S/C12H20O3/c1-6-12(5)8-7-10(15-12)11(3,4)14-9(2)13/h6,10H,1,7-8H2,2-5H3/t1
InchiKey: PZMSWQCFPOWCEC-KFJBMODSSA-N
Formula: C12H20O3
SMILES: C=CC1(C)CCC(C(C)(C)OC(C)=O)O1
Mol. weight [g/mol]: 212.29

Physical Properties

Property code	Value	Unit	Source
gf	-155.85	kJ/mol	Joback Method
hf	-495.75	kJ/mol	Joback Method
hfus	17.62	kJ/mol	Joback Method
hvap	52.80	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.452		Crippen Method
mcvol	178.090	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	1291.00		NIST Webbook
rinpol	1291.00		NIST Webbook
tb	581.50	K	Joback Method
tc	796.30	K	Joback Method
tf	354.95	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.56	J/mol×K	581.50	Joback Method
cpg	486.68	J/mol×K	617.30	Joback Method
cpg	503.67	J/mol×K	653.10	Joback Method
cpg	519.66	J/mol×K	688.90	Joback Method
cpg	534.79	J/mol×K	724.70	Joback Method
cpg	549.18	J/mol×K	760.50	Joback Method
cpg	562.94	J/mol×K	796.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R519436&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume